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DEM FLUIDIZATION OF SMART PARTICLES

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ABSTRACT
Numerical simulations using DEM for smart particles/bodies having a capability to induce a repulsive force on the particle based on the cognition were simulated. A particle-particle interaction type repulsive force was used to induce self fluidization and it was found that if the repulsive force is sufficiently high, fluidization of particles can be achieved.

INTRODUCTION
With the recent advances in particle technology and in nano-technology, and development of micro-scale devices capable of propelling themselves in a controlled way, for instance, by using paramagnetic particles [1] with potential applications to microtechnological [2] and biomedical fields [3,4]. It would thus be just a matter of time that particles having some sensing/recognition capability by their surface modifications and ability to take certain action based on their recognition are developed. If these micro-scale devices possess such a sensing, predicting, judgment and action taking capability they should be called smart micro-bodies. From powder technology view point we may call them smart 'particles'. Investigation of meso and macro scale behavior of such particles would then completely broaden the scope and realms of powder technology and also applications of such particles would become possible in different environments. Although they might be originally designed for some specific tasks, their presence in bulk might show completely different characteristics than their individual presence.

It is thus interesting to study the behavior in bulk behavior of smart particles by using discrete element simulation based on their inter-particle micro interactions. This is because with simulation we can predict and examine their behavior in minute detail prior to design and manufacture of such micro-bodies. In cases where particle to particle repulsion is included in the actions made by these smart micro-bodies, some kind of 'fluidization' should take place in their bulk behavior, which would help manipulation of such bodies in some cases and disturbed in other.

Also in a system of such smart micro-bodies the effect of interstitial gas should be important. Thus we, in the present work, extend out previous work on fluidization via Euler-Lagrangian approach such as, wet fluidized beds (Mikami et al. [5]), heat transfer in fluidized beds (Rong et al. [6]), non isothermal chemical reactions (Kaneko et al. [7]), agglomeration (Iwadate et al. [8]), cohesive interactions and scaling issues (Kuwagi et al. [9]) and by introducing new categories into the particle-to-particle interaction we have so far investigated.

However, the 'smart micro-bodies' and their numerical simulation by Lagrangian manner resembles or equals to the multi agent based simulation (ABS/MABS) that has been popular in

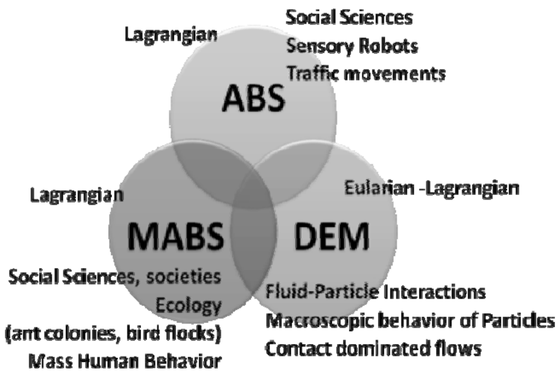

Fig. 1 Venn diagram showing common regions of various simulation techniques

social sciences dealing with the macroscopic, i.e. social effects of agents' individual properties [10]. In ABS models the decision processes of the simulated agents are described at microscopic levels which are then used to understand how the structures emerge at the macroscopic level as a result of the actions of the agents, and their interactions with other agents and the environment. The earliest form of an agent-type work has been implemented dates back to the early 1960s when McPhee studied the modeling of voter behavior [10]. In 1970s, Schelling (1971) [11] studied the housing segregation pattern for neighborhood self-organization in which agents search for neighborhoods with some proportion of similar agents. In the 1980s artificial intelligence and multi agent systems were incorporated in ABS for real-world systems, for biological agents (e.g. bird flocking behavior), referred as artificial life by Reynolds [12] and in mainstream social science for simulation of prisoner's dilemma to study the evolution of cooperation by Axelrod, 1984, [13] . In 1990s ABS was developed for growing artificial societies by a bottom up approach [14,15]. More recently, ABS has been applied to a wide variety of disciplines like social science, for simulations of insect societies, group dynamics in fights, growth and decline of ancient societies, spread of epidemics, etc.; in economics for studying, self organizing markets, trade networks, consumer behavior; in the field of ecology for simulation of, land use dynamics, flocking behavior in fish and birds, rain forest growth and in political science for studying, party competition, origins and patterns of political violence, power sharing in multicultural states [10].

Although ABS has been successfully applied for the study of social systems, as pointed out by Terano, 2006 [16], in social systems, there are no Newton's laws and no first principles. Thus, this makes these approaches both easy and difficult. The easy face is that the models can be made as per one's own will; on the other hand, the difficult face is that the models are hardly grounded in any rigorous grounding theories. Thus, to model a system which follows an intelligent or a smart behavior in an environment where Newton's laws are applicable, like in a system of surface modified particles with ability of taking certain action, a combination of DEM and ABS type of modeling approach needs to be followed as shown in Figure 1.

The objective of this study is to incorporate the decision making capability in the particles by giving the particles capability of recognition of other particles in the vicinity and taking an action based on this recognition to avoid collision with other particles. However, to start from simplest simulations we dis-include capability of prediction which requires memorizing capability. Thus we call the present intelligence as 'smartness'. These microscopic interactions between the smart particles are studied using various parameters to understand the macroscopic behavior of the particles in the bed by inducing self fluidization capability in the bed of particles having these inter-particle interactions to avoid collisions.

MODELING OF SMART PARTICLES

Basic Assumptions for modeling of smart particles

In the present study, since microscopic interactions between the smart particles were studied, it was assumed that the larger sized particles were basically composed of nano-sensors having a laser point vision for optically sensing other particles in the vicinity (Fig. 2) and built in nano-motors with sufficiently high internal battery life for propulsion of the particles based on the surrounding conditions. On detection of another particle in its vicinity, the particle uses its internal energy storing mechanism for propulsion to avoid collision. This smart action as a whole can become similar to passive repulsive force in nature. The existing life bodies are the examples of such smart particles but in the near future artificial robot like bodies could be equipped with such capabilities to actively avoid collisions for their survival. The basic assumptions for the model are listed as follows,

1. The particles are soft spherical balls.
2. The particles are equipped with internal battery which has infinite energy and can be used to generate a force whenever the particle wants to use it.
3. Particles have a limited laser point vision in its direction of velocity.
4. On detection of another particle in its vicinity, the particle uses its internal battery for propulsion to avoid collision. This action is similar to exerting a force of repulsive nature to avoid the collision with the detected particle by using its propulsion system.
5. The repulsive force is a type of surface interaction force. i.e. $F \propto -\frac{1}{\delta^2}$, where, δ is the particle-particle surface distance.

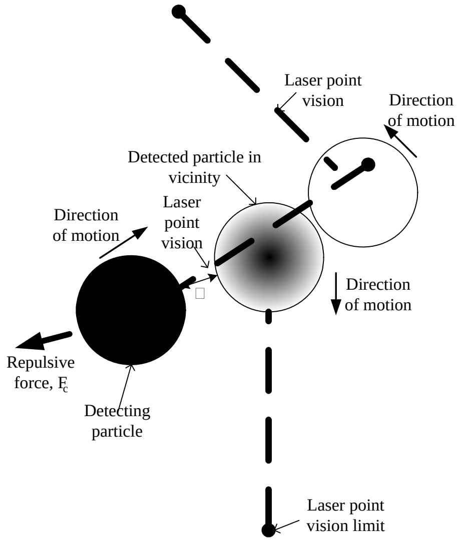

Fig. 2 Detection and action capability concept in smart particles

Modified equation of motion of particles

Motion of each particle is expressed by the Newton's equations of motion as: translational motion:

$$m\frac{dv}{dt} = -V_p \nabla p + F_{fp} - F_{impact} - mg - F_c \quad (1)$$

rotational motion:

$$I\frac{d\omega}{dt} = M_{impact} + M_{wall} + M_{fp} \quad (2)$$

where, F_c[N] is the repulsive recognition force exerted by the particle on itself. Here it should be noted that, the value of F_c is non zero only when a particle is detected in its vicinity otherwise it is zero which is decided by the particle, when there is a particle in vicinity. The governing equations for fluid particle interactions can be found elsewhere [17].

Detection of particles in vicinity

The detection capability of the particles was set as 4 times the radius of particle. This detection capability was a laser point vision in the direction of motion of the particle. The laser point vision was such that, the particle in the immediate vicinity is detected. If there are more than one particle in the vicinity in the direction of motion of the particle, then the particle nearest to it will be detected and corresponding repulsive force would be exerted by the particle on itself to avoid collision with the particle in the vicinity. Since, the simulation is done at interval of each time step, the detection of particle in the vicinity was done at every time interval. The detection of particle in the vicinity is thus valid for the next time step. However, if the particle in vicinity continues to remain in the vicinity, the particle would be continuously detected and the induced repulsive force would be acted upon by the detecting particle as can be seen in Fig. 2.

Repulsive force for fluidization

As any force is inversely proportional to the square of the distance between the particles a generalized force equation was used to induce the fluidization. However, since fluidization is defined as a phenomena that has been used to introduce a phase change in the behavior of solid particles in bulk from a solid phase like behavior to a liquid phase like behavior by introducing a fluid in the bulk solid phase which induces a drag force on the solid bulk phase to counter the internal friction induced due to particles in contact by the gravitational force the repulsive force equal to the weight of the particles (gravitational force) should be sufficient to induce fluidization. However, as not all the particles in the bed would detect other particles in their vicinity, the force required to induce fluidization in the bed should be higher than weight of the particle. Hence, the generalized repulsive force equation was modified as follows,

$$F_c = f\frac{mg}{\delta^2} \tag{3}$$

Where, f is a numerical parameter, which can be changed to increase or decrease the repulsive force for studying the bed behavior and δ is the particle to particle surface distance. To avoid singularity in the above equation, it was assumed that at or below the minimum particle to particle separation distance (1μm) the maximum value of the repulsive force, F_{cmax}, given by

$$F_{cmax} = fmg \tag{4}$$

SIMULATION OF NORMAL PARTICLES AND SMART PARTICLES

Simulation Methodology

For the bed preparation, particles were randomly arranged in the domain and then allowed to settle under gravity without any air flow from bottom. After initializing all the appropriate simulation parameters, the bed voidage and particle surface areas in each fluid cell were calculated. Particle-particle interaction and particle-wall forces were calculated and individual particle positions as well as velocities were obtained by integration, after which fluid dynamics calculations based on the SIMPLE scheme were performed. This procedure was repeated for the entire simulation time, in this case 1s.

Table 1 Simulation conditions

Simulation Conditions (SI units)	
Bed dimensions	
Length	21×10^{-3}
Breadth	10.5×10^{-3}
Height	70×10^{-3}
Particles	
Diameter	10^{-3}
Density	2500
Shape	spherical
Number	2500
Recognition capability	4*R
Parameters	
Normal particles	fluid velocity
Smart particles	repulsive force
Simulation parameter	
Time step	2.5×10^{-5}

Simulation conditions

Eulerian-Lagrangian numerical simulations using a modified drag coefficient for estimating the fluid drag force were performed in a rectangular simulation domain and different cases consisting of varying repulsive forces for mono-dispersed system of normal and smart particles were modeled as summarized in table 1. The coefficient of restitution was set as 0.9.

For the bed preparation, particles were randomly arranged in the domain and then allowed to settle under gravity. After initializing all the appropriate simulation parameters, the bed voidage and particle surface areas were calculated, followed by the computation of the fluid-particle interaction forces.

Particle-particle interaction and particle-wall forces were calculated and the particle positions as well as velocities were obtained by integrating Eqs. (1)&(2), after which fluid dynamics calculations based on the SIMPLE scheme were performed. This procedure was repeated for the entire simulation time of 1s.

The recognition capability of the smart particles was set as 4 times the radius of particle. This recognition capability was a laser point vision in the direction of motion of the particle. The laser point vision was such that, only the particle in the immediate vicinity is detected. If there are more than one particle in the vicinity in the direction of motion of the particle, then the particle nearest to it will be detected and corresponding repulsive force would be exerted by the particle on itself to avoid collision with the particle in the vicinity.

EVALUATION METHODOLOGY

Particle Pressure

To study the condition of fluidization more closely quantitatively, solids pressure for the particles in the bed was calculated [18] from the following equations,

$$\sigma_{i,ab} = \frac{1}{V_i}\sum_{i\neq j} F_a^{ij} r_b^{ij} \tag{5}$$

Where, r_{ij} is the position of the contact point of the force F^{ij} of particle *j* on particle *i*, and *a* and *b* are the Cartesian coordinate components and take the value 1, 2, 3. V_i is the free volume of the particle *i.* The solids pressure can be calculated as,

$$p_i = \frac{1}{3}\sum_{a=1}^{3} \sigma_{i,aa} \tag{6}$$

F_y and bed weight

The bed weight was calculated by summation of the weight of all particles in the bed. The force in vertical direction F_y was summed up for each particle for every time interval, which was calculated as follows,

$$F_y = \sum_{i=1}^{n} (F_{yi}) \tag{7}$$

Probability Density Function

The probability density function (PDF) of solids pressure was calculated by the following formula [19]

$$PDF(p_i) = \frac{\text{number of particles whose solids pressure} \in [p_i, p_i + \Delta p]}{\text{total number of particles } X\ \Delta p} \tag{8}$$

where, Δp is the pressure increment set as 0.04Pa for this case. Eq. (8) gives the instantaneous solids pressure at a particular time. These values of PDF where taken after every 100*Δt to obtain a time-averaged value of PDF, after the particles had settled down (as in the case of gravity settling without fluid injection) i.e. from t=0.5s to t=1s.

RESULTS AND DISCUSSIONS

Fluidization of normal particles with gas injection

To fluidize a bed of particles, as described in the previous section the drag force exerted by the fluid on the particles should counter the internal friction induced due to particles in contact by the gravitational force. Campbell et. al. [20] performed experiments with sand particles and found that particle pressure in the fluidized bed on increasing the gas velocity and as the gas velocity approaches minimum fluidization velocity, the particle pressure in the bed decreases.

Fig. 3 shows the probability density function (PDF) of particles pressures calculated from Eqs. (6)&(8) for normal particles on increasing fluid velocity. From the plot it can be clearly seen that, as the fluid velocity is increased, the height of the PDF function decreased, indicating a reduction in solids pressure on increasing fluid velocity. The PDF function for particle pressure reduced drastically when u_o was

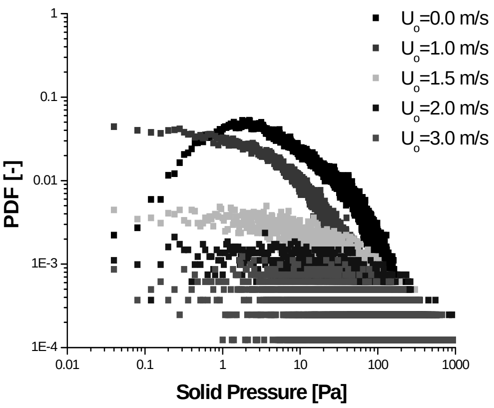

Fig. 3 PDF of solids pressure for normal particles on increasing gas velocity

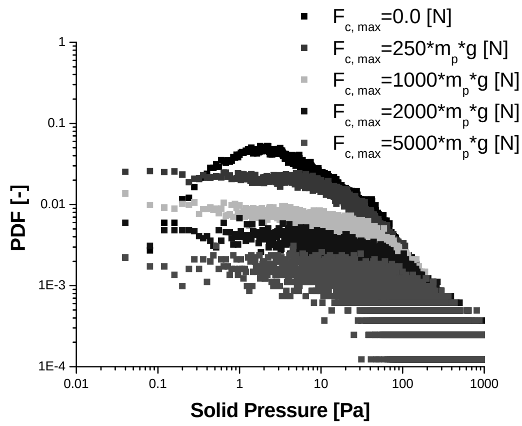

Fig. 4 PDF of solids pressure for smart particles on increasing repulsive force

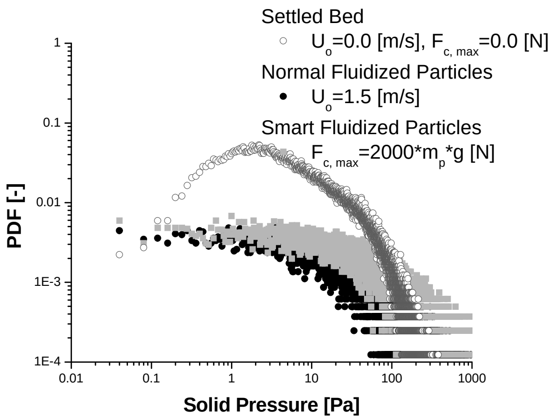

Fig. 5 Comparison of PDF of solids pressure for normal particles and

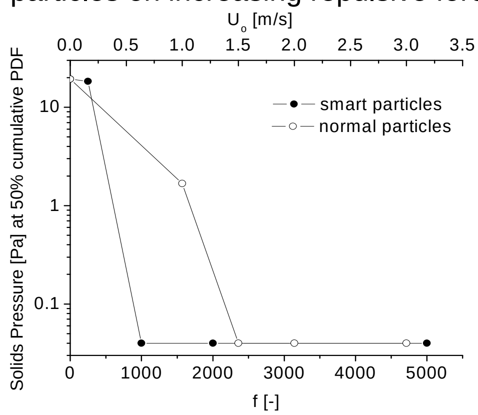

Fig. 6 Comparison of 50% cumulative solids pressure on varying f and U_o for smart and normal particles, respectively.

increased from 1m/s (incipient-fluidized state) to 1.5m/s (fluidized state) and u_{mf} calculated from Wen-Yu equation was obtained to be 0.8m/s for the same particle properties. This clearly agrees with Campbell et. al's results that the fluidization in bed causes reduction of solids pressure.

Fluidization of smart particles without gas injection

Fig. 4 shows the PDF function in the bed of smart particles. In the bed there was no injection of gas from the bottom, the only parameter that was changed was f for increasing the repulsive force exerted by the particle on detection of particle in the vicinity. On changing f in Eq. (3) from the plot it can be seen that as f was increased, the height of PDF function of the solids pressure decreases indicating some sort of fluidization in the bed. The fluidization in the bed is mainly obtained due to the repulsive force induced by the particle on detecting another particle in the vicinity, increasing the value of parameter *f* caused larger repulsive force to be induced by the particles on detection causing the bed to fluidize. The increase of parameter *f* can be thought of as analogous to increasing the fludizing air velocity and reduction in solids pressure indicates fluidization.

Fig. 5 shows the comparison between the PDFs of solids pressure of normal particles in a settled bed and fluidized bed for a fluid velocity of 1.5 m/s (approximately $2U_{mf,WY}$) and smart particles with *f* set as 2000 from the plot it can be seen that the PDFs for the fluidized bed cases is almost similar indicating fluidization in the bed by not introducing gas flow but by the repulsive force exerted by the particle on detection of another particle in the case of smart particles. Fig. 6 shows the comparison for 50% cumulative solids pressure PDF for normal and smart particles, which clearly indicates that as the gas velocity and repulsive forces are increased, the bed of particles attains fluidization and the solids pressure in the bed approaches 0.

The fluidization phenomenon can also be explained by comparing the weight of bed with the summation of forces in vertical direction calculated from Eq. (7) for the case both normal and smart particles. Fig. 7 shows the cumulative repulsive force of all the particles in y-direction. It was found for *f*=250, that the cumulative force in y-direction was lower than the weight of bed, however, for the case of *f*=1000, the total force acting in the y-direction was greater than the weight of the bed and thus, the bed was found to be fluidized. Similarly in the case of normal particles, the bed weight was greater than the drag force exerted by the fluid on the particle in the y-direction due to fluid flow for $U_o=0.4 m/s$, however, for $U_o=1 m/s$ the cumulative drag force induced on the particles in the y-direction was greater than the weight of bed and the bed was found to be fluidized. Interesting thing to note here is the sinusoidal nature of the repulsive force. When the bed is not fluidized, the drag force exerted by the fluid in the y-direction is almost constant, as the particles are in the state of fixed bed condition and the fluid flows through the voidages in the bed. However, when fluidized state is reached, the particle-particle interactions take place, resulting in the sinusoidal nature of the cumulative force in y-direction. On the other hand, in the case of smart particles as the gas is not induced in the bed, the drag force due to fluid is zero, however, since the particles are detecting other particles in their direction of motion, the repulsive force is exerted by the particles, since the repulsive force is a particle-particle force, the nature of cumulative force in y-direction is sinusoidal. Furthermore, as the repulsive force is due to particle-particle interaction, the bubbles or slugs are not formed in the case of smart particles unlike in the case of normal particles because of particle-fluid interactions.

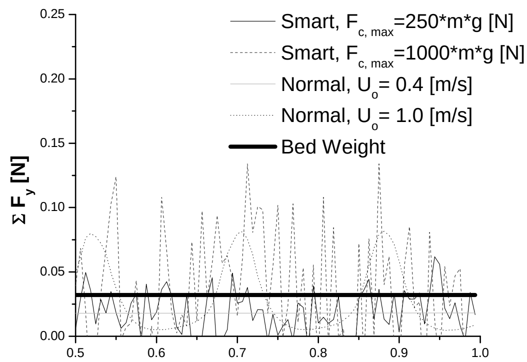

Fig. 7 Comparison of cumulative force in vertical direction for normal particles and smart particles' bed weight

CONCLUSIONS

Numerical simulations using DEM for smart particles/bodies having a capability to induce a repulsive force on the particle based on the cognition were simulated. A particle-particle interaction type repulsive force was used to induce self fluidization and it was found that if the repulsive force is sufficiently high, fluidization of particles can be achieved.

The present research just focuses on introduction of the concept of smart particles and how DEM can be applied for study of behavior of such particles in bulk phase; in the present case only fluidization behavior was considered. However, this kind of research can be applied for many different parameters and their effects be studied on such smart particles which can lead to a new paradigm shift for particulate processes.

NOTATION

d_p	particle diameter [m]		*greek letters*
f	dimensionless numerical parameter for changing repulsive force [-]	$\sigma_{i,aa}$	solid stress of particle *i* in *‘a‘* plane, where ‘*a’* can be 1,2 or 3 corresponding to x, y and z axis [Pa]
F^{ij}	interaction force of particle *j* on particle *i* [N]	δ	particle- particle surface distance [m]
F	force [N]	ω	angular velocity [rad/s]
g	acceleration due to gravity [m/s^2]		Subscripts
I	moment of inertia [kg.m^2]	*c*	recognizing particle
m	mass of particle [kg]	*fp*	fluid-particle interaction
M	moment [kg.m^2/s]	*i,p*	particle
p_i	solid pressure of particle *i* [Pa]	*impact*	impact, particle-particle or particle-wall
V	velocity of particle [m/s]	*wall*	wall
W	weight of bed [N]	*n*	number of particles

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